OptiDis: A parallel Fast Multipole Dislocation Dynamics code

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ABSTRACT

Among all the steps involved in DD simulations, the computation of the internal elastic forces and energy are by far the most resources consuming. However, since these are long-ranged and fast decreasing interactions, hierarchical algorithms like the Fast Multipole Method (FMM) are well suited for their fast evaluation.
The relatively low accuracy required for the interaction forces between dislocations brought us to develop a more efficient approximation method for the farfield. On the other hand, the nearfield interactions are still evaluated analytically, which required a rather performant implementation (AVX, GPU...).

Regarding parallelism, our code benefits from a hybrid OpenMP/MPI paradigm and a cache-conscious datastructure. Finally, an accurate handling of topological elements intersecting the structure of the octree was considered. The latter feature implied careful modifications of the P2M/L2P operators in order to deal with shared memory model of parallelism.

MODEL

The motion of dislocations is ruled by a prescribed mobility law (e.g. viscous glide) depending on the internal (i.e. created by dislocations themselves) and external (i.e. applied by user) contributions on the nodal forces.
The isotropic elastic stress field created by a dislocation loop $(\mathbf{b}', \mathbf{t}')$ at point $\mathbf{x}$ in space is given by Mura's formula [4]

$$\sigma_{ij}(\mathbf{x}) = \frac{\mu}{8\pi}((A_{ij})(\mathbf{x}) + (A_{ji})(\mathbf{x}) + \frac{2}{1-\nu}(B_{ij} - \delta_{ij}B_{pp})(\mathbf{x}))$$

where (μ, ν) are the Lamé coefficients and

$$(A_{ij})(\mathbf{x}) = \oint_{(C')} R_{,ppm}(\mathbf{x},\mathbf{y})\varepsilon_{jmk}b'_k t'_i dy \qquad (B_{ij})(\mathbf{x}) = \oint_{(C')} R_{,ijm}(\mathbf{x},\mathbf{y})\varepsilon_{nmk}b'_k t'_n dy$$

with $R(\mathbf{x},\mathbf{y}) = |\mathbf{x}-\mathbf{y}|$. The nodal force $\mathbf{f}^e_n$ acting at the extremities of a finite dislocation line $(\mathbf{b}, \mathbf{t})$ is obtained by integration of the Peach-Koehler force ($\mathbf{f}^{PK} = (\boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{b}) \times \mathbf{t}(\mathbf{x})$) over the target line, i.e.

$$(f^e_n)_\alpha = \oint_{(C)} \varepsilon_{\alpha\beta\gamma}\sigma_{\beta p}b_p t_\gamma N_n(\mathbf{x})dx$$

where $N_{n=1,2}$ are linear shape functions. While the isotropic elastic interaction energy is given by

$$E(C', C) = -\frac{\mu}{8\pi}\oint_{(C)}\oint_{(C')} R_{,kk}(b'_i dx'_i b_j dx_j - \frac{2\mu}{1-\nu}(b'_i dx'_j b_i dx_j - b'_j dx'_i b_i dx_j)) + R_{,ij}\frac{2\mu}{1-\nu}b'_j dx'_k b_i dx_k$$

The cost of updating the nodal forces (and the energy) at each time step is quadratic and involves the evaluation of 2 line integrals, therefore it is usually the bottleneck of DD simulations.

A NEW FFT-ACCELERATED FMM

Fast Multipole DD

The idea of the FMM is to balance the computational cost of near and farfield interactions by approximating the farfield and rely on a tree structure (see figure 1) to perform all computations. In our case we consider the interaction potential $\mathbf{R}(\mathbf{x},\mathbf{y}) = \{R_{,ij}(\mathbf{x},\mathbf{y})\}_{i,j=1..3}$ and apply the interpolation formula

$$\mathbf{R}(\mathbf{x},\mathbf{y}) \approx \sum_{|\boldsymbol{\alpha}|\leq p} S_{\boldsymbol{\alpha}}(\mathbf{x}) \sum_{|\boldsymbol{\beta}|\leq p} \mathbf{R}(\bar{\mathbf{x}}_{\boldsymbol{\alpha}}, \bar{\mathbf{y}}_{\boldsymbol{\beta}})S_{\boldsymbol{\beta}}(\mathbf{y})$$

where $\bar{\mathbf{x}}_{\boldsymbol{\alpha}}$ and $\bar{\mathbf{y}}_{\boldsymbol{\beta}}$ denote 2 sets of interpolation nodes in 2 well separated clusters containing $\mathbf{x}$ and $\mathbf{y}$. S denotes a polynomial interpolator (either Lagrange or Chebyshev).

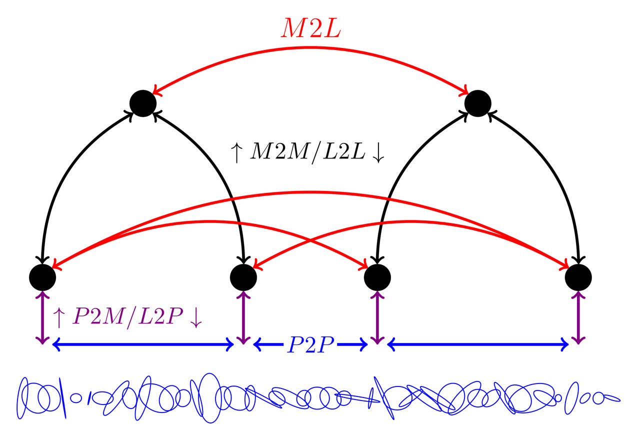


FIGURE 1: Tree structure with operators.

The farfield approximation consists in 3 steps:
$P2P$ Analytical evaluation of the nearfield.

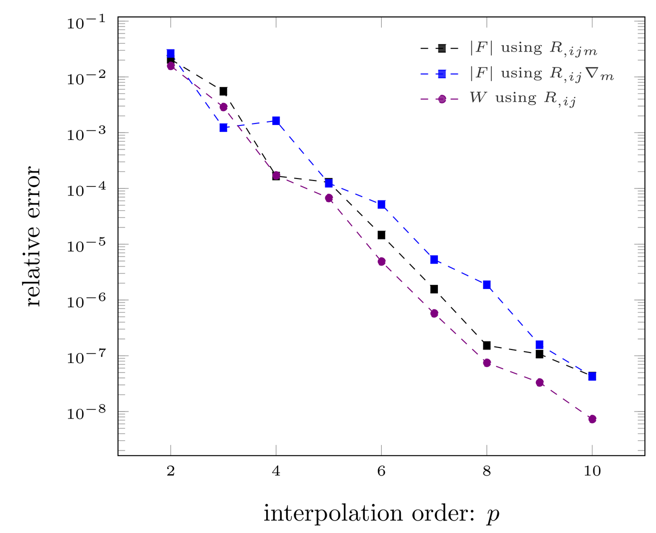
$P2M/L2P$ Integration of polynomial interpolators on all leaf cells returns expansion:

$$\mathcal{M}_{\boldsymbol{\beta}} = \oint_{(C)} S_{\boldsymbol{\beta}}(\mathbf{y})dy$$

$M2M/L2L$ Transfer expansions between levels.
$M2L$ Transfer expansions between cells in interaction by applying

$$\mathcal{L}_{\boldsymbol{\alpha}} = \mathbf{R}_{\boldsymbol{\alpha\beta}}S_{\boldsymbol{\beta}}$$

Both stress and energy expansions share the same M2L operators $\mathbf{R}_{\boldsymbol{\alpha\beta}}$, but the extra derivation involved in the stress field is applied to the interpolator. This results in a slightly lower accuracy but less M2L operations to be performed (see figure 2).



Approach	$\mathcal{O}_t^F$	$\mathcal{O}_t^W$	$\mathcal{O}_m^{F+W}$
$R_{,ijm}$	45	–	$10+6$
$R_{,ij}\nabla_m$	21	36	6
$(R_{,ij}\|R_{,pp})\nabla_m$	12	36	7

FIGURE 2: Accuracy of various FMM schemes (left) and their relative costs (right).

Acceleration by Fast Fourier Transform (FFT)

Even though the Chebyshev-based FMM [3] provides a very accurate algorithm it is very expensive in terms of memory and CPU time, namely $\mathcal{O}(p^6)$ for the M2L step. Thus a new interpolation scheme based on an equispaced grid (Lagrange) was considered. In this approach $R_{\boldsymbol{\alpha\beta}}$ is Toeplitz since $\mathbf{R} = \mathbf{R}(|\mathbf{x}-\mathbf{y}|)$. As illustrated below, $R_{\boldsymbol{\alpha\beta}}$ can be seen as a convolution and applied in Fourier space with a linear cost.

If R$=\begin{bmatrix} a & b & c \\ d & a & b \\ e & d & a \end{bmatrix}$, then RX=$FFT^{-1}(FFT(C_0) : FFT(X))$ with $C_0 = \begin{bmatrix} a & b & c & e & d \end{bmatrix}$

The scheme remains stable and sufficiently accurate in the scope of DD simulations (min. accuracy on force computation $\approx 10^{-3}$), while dramatically decreasing the computational cost of the M2L, namely to $\mathcal{O}((2p-1)^3)$. Let $p=5$ then in double precision the memory required for the M2L equals:

$$316 \times (2\times 5-1)^3 \times 7 \times (2\times 8) \approx \underline{25 \text{ MBytes}}$$

IMPLEMENTATION AND PERFORMANCES

Our experimentations were performed on the core program OptiDis whose data structure relies heavily on the open source ScalFMM library [1]. The latter also provides the generic Fast Multipole algorithms. OptiDis implements its own dislocation specific P2M/L2P routines involving exact integration over segments as well as analytic expressions for nearfield taken from Arsenlis et al [2].

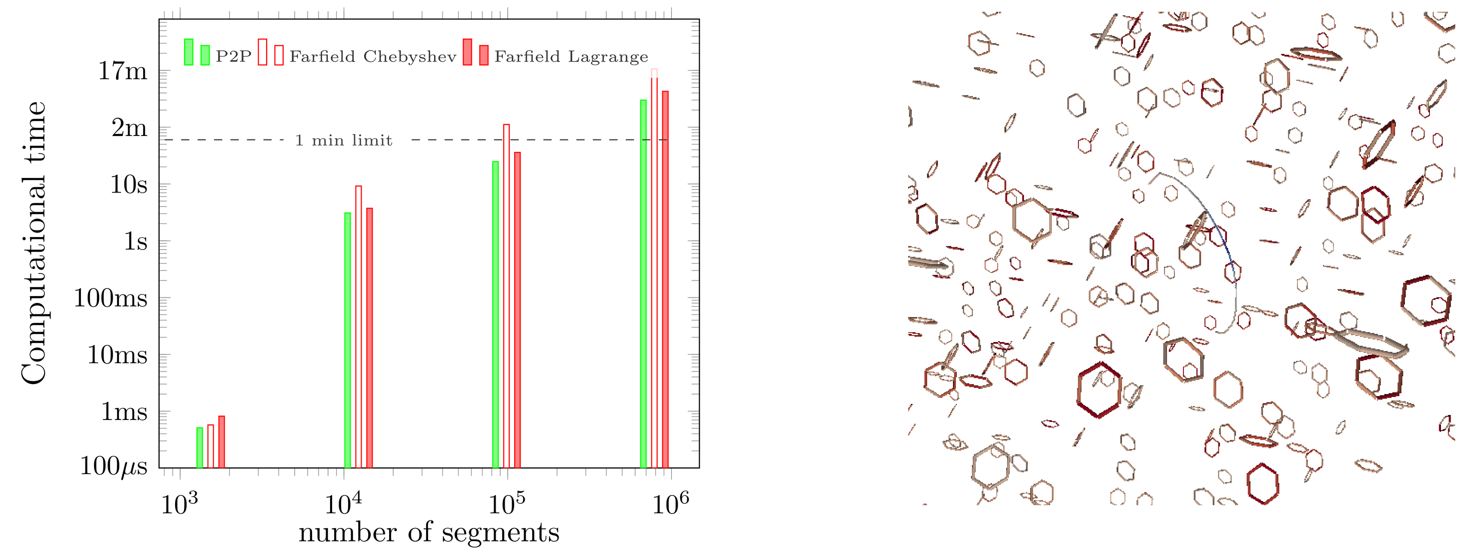


FIGURE 3: Near- and Farfield computational time balancing for a uniform distribution of dislocation loops and increasing tree depth (left). An example of defects distribution and a propagating Frank-Read source (right).

ZR: CLEAR BAND CHANNELS

One of the main goals of OptiDis project was to simulate the formation of clear band channels in Zirconium. Therefore we considered many defects (dislocation loops) located either in the basal or the prismatic plane and activated the motion of many Frank-Read sources ($b =< 1, 1, -2, 0 >$) by applying an external stress state to the grain ($\approx 100MPa$).

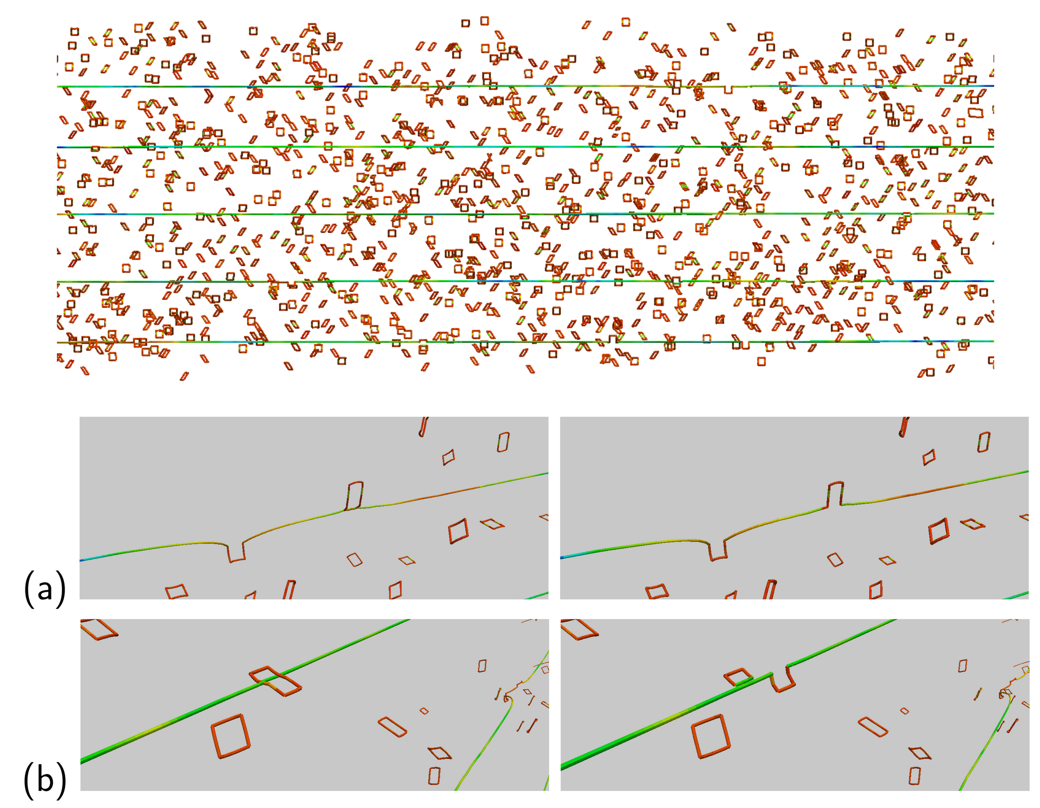


FIGURE 4: Evolution of 6 screw Frank-Read sources (top) inside a grain of Zr with a large density of defects ($d = 1.10^{22}m^{-3}$). Elementary events (bottom): (a) double jog (b) dissociation.

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